

Propane, 1,1'-sulfonylbis[2-methyl-

Other names:	(iso-C4H9)2SO2 1,1'-Sulphonylbis(2-methyl-propane) Diisobutyl sulfone Diisobutyl sulphone Isobutyl sulfone Propane, 1,1'-sulfonylbis*2-methyl-
Inchi:	InChI=1S/C8H18O2S/c1-7(2)5-11(9,10)6-8(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	ULSLZZKKTPQNNJ-UHFFFAOYSA-N
Formula:	C8H18O2S
SMILES:	CC(C)CS(=O)(=O)CC(C)C
Mol. weight [g/mol]:	178.30
CAS:	10495-45-1

Physical Properties

Property code	Value	Unit	Source
chl	-5697.69 ± 0.59	kJ/mol	NIST Webbook
hf	-535.60 ± 2.60	kJ/mol	NIST Webbook
hfl	-625.17 ± 0.84	kJ/mol	NIST Webbook
hfus	20.81	kJ/mol	Joback Method
hvap	90.00 ± 3.00	kJ/mol	NIST Webbook
ie	9.54 ± 0.05	eV	NIST Webbook
logp	1.713		Crippen Method
mcvol	151.670	ml/mol	McGowan Method
tb	538.00	K	NIST Webbook
tb	374.00 ± 3.00	K	NIST Webbook
tf	290.00	K	NIST Webbook
tf	290.10 ± 0.60	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.59	J/mol×K	429.34	Joback Method
cpg	323.91	J/mol×K	457.50	Joback Method
cpg	337.72	J/mol×K	485.67	Joback Method

cpg	351.02	J/mol×K	513.83	Joback Method
cpg	363.80	J/mol×K	541.99	Joback Method
cpg	376.08	J/mol×K	570.15	Joback Method
cpg	387.85	J/mol×K	598.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49079e+01
Coeff. B	-4.60194e+03
Coeff. C	-9.07560e+01
Temperature range (K), min.	405.52
Temperature range (K), max.	570.30

Sources

The Yaws Handbook of Vapor Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C10495451&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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